



>>Entry Name: 4-Methyl-1-pentanol, 9CI

Synonym(s): Isohexanol

CAS Registry Number: 626-89-1

$(\text{H}_3\text{C})_2\text{CHCH}_2\text{CH}_2\text{CH}_2\text{OH}$

Molecular Formula: $\text{C}_6\text{H}_{14}\text{O}$

Molecular Weight: 102.176

Accurate Mass: 102.104465

Percentage Composition: C 70.53%; H 13.81%; O 15.66%

Boiling Point: Bp 152-153°

Density: d_4^{25} 0.811

Refractive Index: n_D^{25} 1.4134

Aldrich: M6695-1

Fluka: 68430

>>Derivative: *O*-[α -D-Galactopyranosyl-(1→6)- β -D-galactopyranoside]

Synonym(s): Capsoside B

Molecular Formula: $\text{C}_{18}\text{H}_{34}\text{O}_{11}$

Molecular Weight: 426.46

Accurate Mass: 426.210115

Percentage Composition: C 50.70%; H 8.04%; O 41.27%

Biological Source: Constit. of the fruit of *Capsicum annuum* var. *acuminatum*

Optical Rotation: $[\alpha]_D^{25}$ -17 (c, 0.07 in MeOH)

>>Derivative: Ac

CAS Registry Number: 628-95-5

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2$

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Boiling Point: Bp₁₅₅ 159°

>>Derivative: 3,5-Dinitrobenzoyl

Melting Point: Mp 70°

>>Derivative: Benzenesulfonyl

Molecular Formula: $\text{C}_{12}\text{H}_{18}\text{O}_3\text{S}$

Molecular Weight: 242.338

Accurate Mass: 242.097665

Percentage Composition: C 59.48%; H 7.49%; O 19.81%; S 13.23%

Boiling Point: Bp₇ 170°

References:

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